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TITLE: SIMULATIONS OF THE ASCOT BRUSH CREEK DATA BY A NESTED-GRID, SECOND-MOMENT TRUBULENCE-CLOSURE MODEL AND A KERNEL CONCENTRATION ESTIMATOR

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SIMULATIONS OF THE ASCOT BRUSH CREEK DATA BY A NESTED-GRID, SECOND-MOMENT TURBULENCE-CLOSURE MODEL AND A KERNEL CONCENTRATION ESTIMATOR

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1. INTRODUCTION

Yamada and Bunker (1986) demonstrated that a three-dimensional hydrodynamic model, HOTMAC, (Higher Order Turbulence Model for Atmospheric Circulations) reproduced nocturnal drainage flows, morning transition and convective upvalley and upslope flows observed during the 1982 ASCOT (Atmospheric Studies in COmplex Terrain) field campaign in Brush Creek, Colorado. We also showed that a Monte Carlo statistical diffusion model, RAPTAD (RAndom Particle Transport And Diffusion) driven by the outputs (mean and turbulence variables) from HOTMAC simulated well the structure of an SF_6 tracer plume and obtained a vertical profile of concentration similar to the one observed.

In the previous studies (Yamada, 1981 and 1985; Yamada and Bunker, 1986), the concentration at a given time and location was determined by counting the number of particles in an imaginary sampling volume. The computed concentration level could vary considerably depending on the size of the sampling volume and number of particles used in the computation. For example, if the sampling volume is very small, the concentration distribution becomes very noisy. On the other hand, if the sampling volume is too large, the concentration distribution is oversmoothed. Theoretically, the sampling volume problem is eliminated by releasing an infinite number of particles in the computation. Of course, it is impossible in practice, or at least very expensive, to release an infinite number of particles.

A "kernel" density estimator is used in this study where each particle represents a center of a puff. Various functional forms may be assumed to express the concentration distribution in the puff. One of the simplest ways is to assume a Gaussian distribution where variances are determined as the time integration of the velocity variances encounterd over the history of the puff. The concentration level at a given time and space is determined as the sum of the concentrations each puff contributes. The kernel method requires no imaginary sampling volumes and produces a smooth concentration distribution with a much smaller number of particles than required for the previous particle method.

2. RAPTAD (RAndom Particle Transport And Diffusion)

A brief description of RAPTAD is given here.

Locations of particles are computed from

$$x_i(t+\Delta t) = x_i(t) + U_{pi}\Delta t \quad , \tag{1}$$

where

$$U_{pi} = U_i + u_i \quad , \tag{2}$$

$$u_i(t + \Delta t) = a u_i(t) + b\sigma_{u_i}\zeta + \delta_{i3}(1-a)t_{Lx_i}\frac{\partial}{\partial x_i}(\sigma^2_{u_i}) \quad , \tag{3}$$

$$a = \exp(-\Delta t/t_{Lx_i}) \quad , \tag{4}$$

and

$$b = (1 - a^2)^{1/2} \quad . \tag{5}$$

In the above expressions, U_{pi} is the particle velocity in x_i direction, U_i mean velocity, u_i turbulence velocity, ζ a random number from a Gaussian distribution with zero mean and unit

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variance, t_{Lx_i} the Lagrangian integral time for the velocity u_i, σ_{u_i} standard deviation of velocity fluctuation u_i, and δ_{ij} is the Dirac delta. The last term on the right-hand side of Eq. (3) was introduced by Legg and Raupach (1982) in order to correct accumulation of particles in inhomogeneous turbulent flows. The mean velocity U_i and standard deviation of velocity σ_{u_i} are obtained from a hydrodynamic model, HOTMAC.

3. KERNEL DENSITY ESTIMATOR

Concentration χ at (X, Y, Z) is estimated by using the following expression:

$$\chi(X, Y, Z) =$$

$$\frac{Q\Delta t}{(2\pi)^{3/2}} \sum_{k=1}^{N} \frac{1}{\sigma_{x_k}\ \sigma_{y_k}\ \sigma_{z_k}} \exp(-\frac{1}{2}\frac{(x_k - X)^2}{\sigma_{x_k}^2})$$

$$\bullet \exp(-\frac{1}{2}\frac{(y_k - Y)^2}{\sigma_{y_k}^2})$$

$$\bullet(\exp(-\frac{1}{2}\frac{(z_k - Z)^2}{\sigma_{z_k}^2}) +$$

$$\exp(-\frac{1}{2}\frac{(z_k + Z - 2\ z_g)^2}{\sigma_{z_k}^2})) \quad , \quad (6)$$

where (x_k, y_k, z_k) is the location of k th particle; σ_{x_k}, σ_{y_k} and σ_{z_k} are standard deviations of a Gaussian distribution; and z_g is the ground elevation. The variances are estimated based on Taylor's (1921) homogeneous diffusion theory. For example, σ_y is obtained from

$$\sigma_y^2 = 2\sigma_v^2 \int_0^t \int_0^\zeta R(\zeta)d\zeta dt =$$

$$2\sigma_v^2\ t_{Ly}(t + t_{Ly} \exp(-\frac{t}{t_{Ly}}) - t_{Ly}) \quad , \quad (7)$$

where a correlation function $R(\zeta) = \exp(\frac{-\zeta}{t_{Ly}})$ is used. Equation (7) is approximated by

$$\sigma_y = \sigma_v\ t \quad \text{for } t \le 2t_{Ly} \quad , \quad (8a)$$

and

$$\sigma_y^2 = 2t_{Ly}\ \sigma_v^2\ t \quad \text{for } t > 2t_{Ly} \quad . \quad (8b)$$

Although the turbulence field in general is not homogeneous, we assume the theory is applicable over a short time period, such as an integration time step (10 sec. in this study). Therefore,

$$\sigma_y\ (t + \Delta t) = \sigma_y\ (t) + \sigma_v \Delta t \text{ for } t \le 2t_{Ly} \quad , \quad (9a)$$

and

$$\sigma_y^2\ (t + \Delta t) = \sigma_y^2\ (t) + 2t_{Ly}\ \sigma_v^2\ \Delta t \text{ for } t > 2t_{Ly} \quad , \quad (9b)$$

are used in this study.

In a similar fashion,

$$\sigma_x\ (t + \Delta t) = \sigma_x\ (t) + \sigma_u \Delta t \text{ for } t \le 2t_{Lx} \quad , \quad (10a)$$

$$\sigma_x^2\ (t + \Delta t) = \sigma_x^2\ (t) + 2t_{Lx}\sigma_u^2 \Delta t \quad \text{for } t > 2t_{Lx} \quad , \quad (10b)$$

$$\sigma_z\ (t + \Delta t) = \sigma_z\ (t) + \sigma_w \Delta t \quad \text{for } t \le 2t_{Lz} \quad , \quad (11a)$$

and

$$\sigma_z^2\ (t + \Delta t) = \sigma_z^2\ (t) + 2t_{Lz}\sigma_w^2 \Delta t \text{ for } t > 2t_{Lz}, \quad (11b)$$

where the standard deviations σ_u, σ_v and σ_w at each particle location are obtained by interpolation of grid values.

4. COMPARISON WITH ANALYTIC SOLUTION

We have selected a hypothetical condition in order to test the accuracy of a RAPTAD kernel density estimator. Under the assumption that the wind and turbulence distributions are homogeneous, concentration χ (X,Y,Z) from a point source is described by a Gaussian distribution:

$$\chi = \frac{Q}{2\pi\ \sigma_y \sigma_z\ U} \exp\left[-\frac{1}{2}\left\{\left(\frac{y}{\sigma_y}\right)^2 + \left(\frac{z}{\sigma_z}\right)^2\right\}\right] \quad , \quad (12)$$

where Q is an emission rate (g/s), U mean wind speed (m/s); σ_y and σ_z standard deviations in the y and z directions, respectively.

The concentration in the horizontal plane at the source height is given from Eq. (12) as

$$\chi = \frac{Q}{2\pi\sigma_y\ \sigma_z\ U}\ \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \quad . \qquad (13)$$

Assuming σ_v = 2 m/s, the variance σ_y is computed from Eq. (7) where t_{Ly} = 10000 s is used. σ_z is similarly computed where σ_w = 0.02 m/s and t_{Lz} = 20 s are assumed. Horizontal wind speed U = 10 m/s is also assumed. The concentration distribution ($\log_{10}\chi$) is shown in Fig. 1.

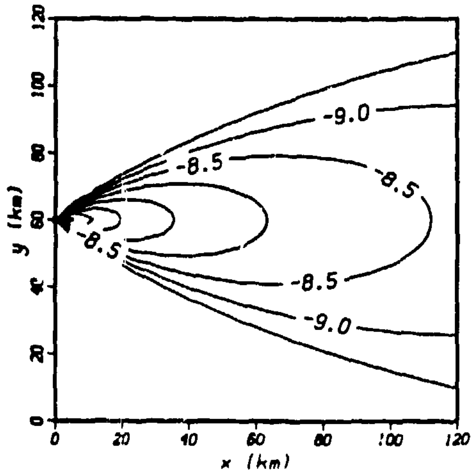

Fig. 1. Gaussian plume concentration distribution on the horizontal plane at a source height. Concentration χ (g/m^3) is given in terms of $\log_{10}$ (χ) where the source emission rate is 1 g/s.

Now we apply RAPTAD under the same meteorological conditions, i.e., U = 10 m/s, σ_v = 2 m/s, t_{Ly} = 10000 s, σ_w = 0.02 m/s, and t_{Lz} = 20 s. In addition, σ_u = 1 m/s and t_{Lx} = 10000 s are assumed. We released 1 particle per 10 s and computed particle locations every 10 s using Eqs. (1) through (5). A total of 2000 particles were released and the particle distributions in a 120 x 120 km^2 domain is shown in Fig. 2. First, the concentrations were determined by counting the number of particles in equal volume boxes in the computation domain. The volume of each box was 2 km x 2 km x 200 m. The concentration distribution is very noisy (Fig. 3) indicating the sampling volume is too small and

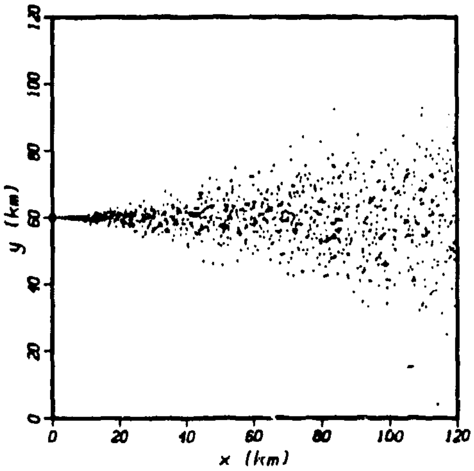

Fig. 2. Distribution of 1,200 particles projected on the horizontal plane at a source height.

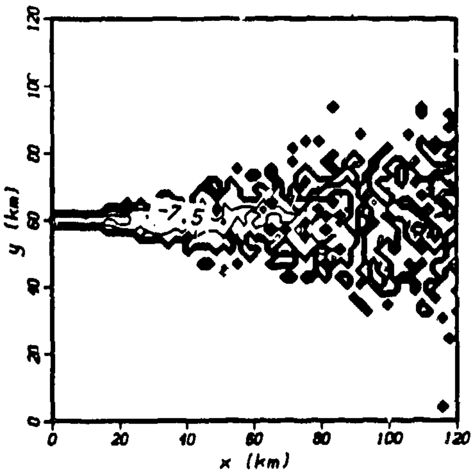

Fig. 3. Concentration distribution obtained by counting the numer of particles in sampling boxes of 2 km x 2 km x 200 m. Concentration contours and emission rate as in Fig. 1.

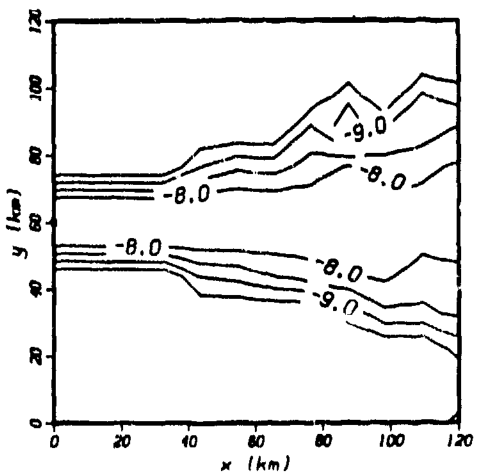

Fig. 4. Same as for Fig. 3 except the sampling boxes are 10 km x 10 km x 200 m.

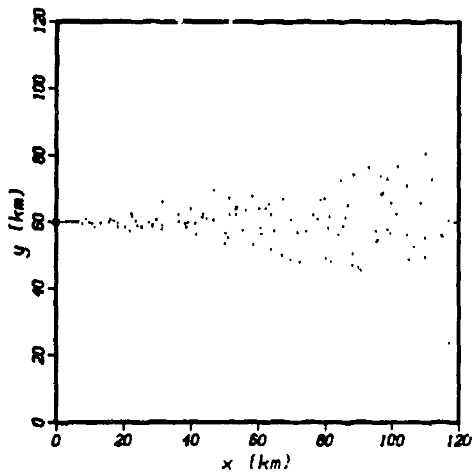

Fig. 5. Distribution of 120 particles projected on the horizontal plane at a source height.

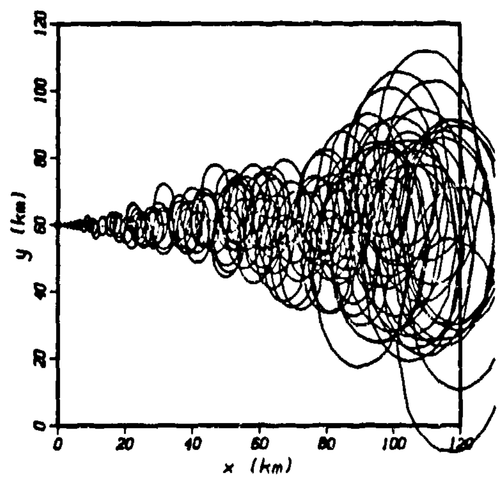

Fig. 6. Distribution of puffs, represented by ellipses of $\sigma_x \times \sigma_y$, centered at particle locations shown in Fig. 5.

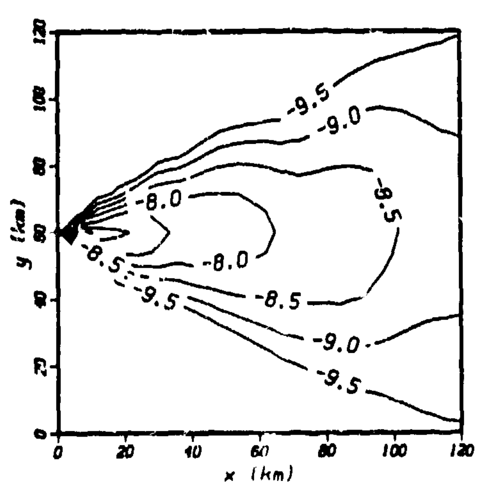

Fig. 7. Concentration distribution obtained by a kernel method. Concentration contours and emission rate as in Fig. 1.

the number of particles released is not large enough. When the sampling volume was enlarged to 10 km x 10 km x 200 m, the concentration distribution was oversmoothed (Fig. 4), particularly in the regions near the source where a plume was very narrow.

The problems associated with the sampling volume and number of particles released are greatly reduced when the kernel density estimator is introduced to calculate concentration values. Figure 5 shows the locations of particles and Fig. 6 the puffs represented by ellipses of $\sigma_x \times \sigma_y$ centered at particle locations. Only 121 particles are used, yet the concentration distribution (Fig. 7) is very similar to the analytical solution (Fig. 1). If the number of particles is increased by a factor of ten, the contour lines (not shown) become smoother but essentially the same as those shown in Fig. 7.

5. BRUSH CREEK DATA SIMULATION

Yamada and Bunker (1986) discussed in detail the 1982 ASCOT Brush Creek experiment, the hydrodynamic model (HOTMAC), and development of nocturnal drainage flows. The HOTMAC outputs and a diffusion code, RAPTAD were used to simulate the SF_6 tracer data. A total of 9,000 particles were released and concentration was obtained by counting the number of particles in an imaginary box of 50 m cube.

In this study, the concentration was recomputed by applying the Gaussian kernel estimator discussed in Section 3. A total of only 900 particles were released. The vertical profile of the modeled SF_6 concentration averaged over one hour between 6 a.m. and 7 a.m. at a site near the mouth of Brush Creek is compared with observation (Fig. 8). The modeled and observed concentrations agree well although the modeled values are slightly smaller than the observations for the first 250 m above the ground. The model overestimates the concentrations in the higher elevations since puffs are assumed to diffuse in horizontal directions rather than in directions parallel and perpendicular to the puff movement. A simple constraint imposed on σ_y<100 m corrected most of the problem.

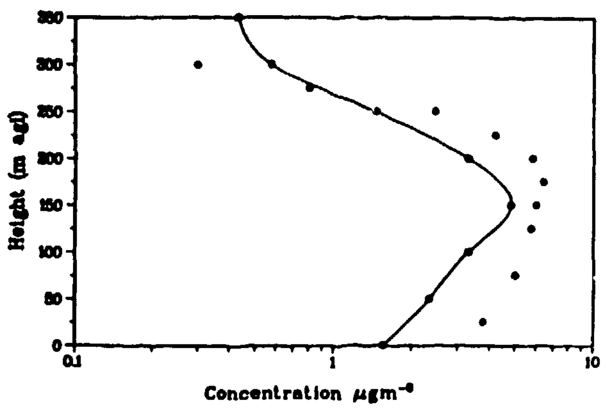

Fig. 8. Vertical profiles of the modeling (- 0 -) and observed (●) SF_6 concentration at SNL site. The values are averaged over an hour between 6 a.m. and 7 a.m.

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